# Effect of measurement probes upon the conductance of an interacting nano-system: Detection of an attached ring by non local many body effects

Axel Freyn and Jean-Louis Pichard
*Service de Physique de l'État Condensé (CNRS URA 2464), DSM/DRECAM/SPEC, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France*

We consider a nano-system connected to measurement probes via leads. When a magnetic flux is varied through a ring attached to one lead at a distance $L_c$ from the nano-system, the effective nano-system transmission $|t_s|^2$ exhibits Aharonov-Bohm oscillations if the electrons interact inside the nano-system. These oscillations can be very large, if $L_c$ is small and if the nano-system has almost degenerate levels which are put near the Fermi energy by a local gate.

PACS numbers: 71.10.-w,72.10.-d,73.23.-b

To map the low temperature behavior of an interacting system onto that of an effective non interacting system with renormalized parameters is the basis of the simplest many body theories (Hartree-Fock (HF) approximation [1], Landau theory of dressed quasi-particles). In one dimension (1d), this mapping fails to describe the collective excitations of a macroscopic wire (Luttinger-Tomonaga limit), but can be used if the electrons interact only inside a microscopic part of a very long wire. This corresponds [2] to the set-up used for measuring the quantum conductance $g$ of a nano-system with two attached probes. The electrons can strongly interact inside the nano-system (molecule, quantum dot with a few electrons, atomic chains created in a break junction) while their interaction can be neglected outside. If the many body scatterer can be mapped onto an effective one body scatterer, detecting the presence of interactions from a zero temperature transport measurement looks difficult. Fortunately, the interactions give rise to a new phenomenon which does not exist in a bare one body scatterer: the effective transmission $|t_s|^2$ ceases [3, 4] to be local. We study in this letter a set-up for detecting by a conductance measurement the non locality of $|t_s|^2$ due to nano-system interactions.

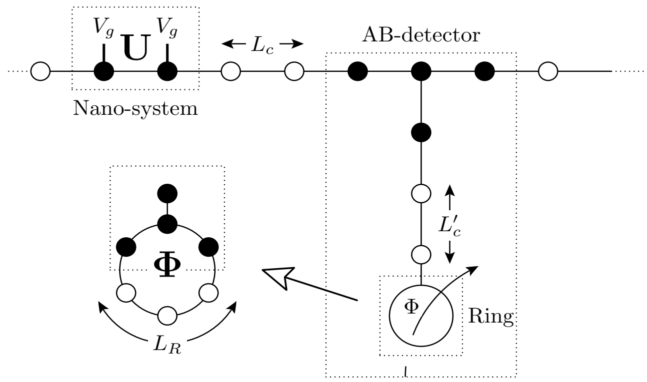


FIG. 1: Considered set-up made of a many body scatterer with two semi-infinite 1d leads: Polarized electrons interact only inside the nano-system (two sites with inter-site repulsion $U$, hopping term $t_d$ and applied gate voltage $V_G$). A ring is attached at a distance $L_c$ from the nano-system.

The idea can be simply explained using the HF approximation [1] and the Landauer formulation [2] of quantum transport. Let us assume a nano-system with interactions in contact with two 1d non interacting leads. Using the HF approximation, one can map the ground state of this set-up onto that of an effective one body scatterer with leads, introducing HF corrections which probe energy scales much below the Fermi energy and length scales much larger than the nano-system size. Via the conduction electrons, one can induce Friedel oscillations of the electron density inside the nano-system by inserting a second scatterer in one lead at a distance $L_c$ from the nano-system. These oscillations change the Hartree and Fock terms of the nano-system effective Hamiltonian. This generates a non local effect upon its effective transmission $|t_s|^2$, and hence upon the Landauer conductance of a set-up embedding the nano-system. This non local effect upon $|t_s|^2$ decays as $1/L_c$ with $\pi/k_F$ oscillations ($k_F$ being the Fermi momentum), if it is driven by Friedel oscillations in 1d leads ($1/L_c^d$ decay for d-dimensional leads). This phenomenon is reminiscent of the RKKY interaction [5] between magnetic moments via conduction electrons. At a temperature $T \neq 0$, this non local effect is exponentially suppressed [4] when $L_c$ exceeds $L_T$, the scale on which the electrons propagate at the Fermi velocity during a time $\propto 1/T$.

We use a simple 1d toy model of polarized electrons (spinless fermions) for which the Hartree-Fock approximation allows to describe [4] the effect of a repulsion $U$ acting between two consecutive sites only. To detect how the nano-system effective transmission $|t_s|^2$ depends on the measurement probes, we put a second (one body) scatterer in one of the leads at a distance $L_c$ from the nano-system. Hereafter, we refer to this second scatterer as the AB-detector, since it includes a ring threaded by an Aharonov-Bohm (AB) flux $\Phi$, the combined set-up being sketched in FIG. 1. Flux dependent Friedel oscillations of the electron density are induced inside the nano-system by the AB-detector. If the electrons interact inside the nano-system, $|t_s|^2$ exhibits periodic AB-oscillations, which vanish if the ring is too far from the nano-system or if the electrons cease to interact.

Our toy model is a tight-binding model on an infinite 1d lattice, where spinless fermions do not interact, unless they occupy the nano-system (two central sites 0 and 1), which costs an energy $U$. A potential $V_G$ can be varied inside the nano-system by a local gate. The Hamiltonian of the nano-system with the leads reads:

$$H = V_G\,(n_1 + n_0) + U n_1 n_0 - \sum_{p=-\infty}^{\infty} t_{p,p-1}(c_p^\dagger c_{p-1} + h.c.). \tag{1}$$

Outside the nano-system, the energy scale is set by a uniform hopping amplitude $t_{p,p-1} = 1$. Inside the nano-system, the hopping amplitude $t_{1,0} = t_d$ is one of the nano-system parameters. $c_p$ ($c_p^\dagger$) is the annihilation (creation) operator at site $p$, and $n_p = c_p^\dagger c_p$. In the HF approximation, the ground state is assumed to be a Slater determinant of one-body wave-functions $\psi_\alpha(p)$ of energy $E_\alpha < E_F$, $E_F = -2\cos k_F$ being the Fermi energy. The effective HF Hamiltonian corresponds to two central sites without nearest neighbor repulsion, with renormalized potentials $V_0$ and $V_1$ (instead of $V_G$) and hopping amplitude $v$ (instead of $t_d$), coupled to two semi-infinite leads. Denoting $\langle c_n^\dagger c_m\rangle = \sum_{E_\alpha<E_F} \psi_\alpha^*(n)\psi_\alpha(m)$, the HF parameters $v, V_0$ and $V_1$ are given by the three coupled equations

$$v = \; t_d + U\left\langle c_0^\dagger c_1(v, V_0, V_1)\right\rangle \tag{2}$$

$$V_0 = \; V_G + U\left\langle c_1^\dagger c_1(v, V_0, V_1)\right\rangle \tag{3}$$

$$V_1 = \; V_G + U\left\langle c_0^\dagger c_0(v, V_0, V_1)\right\rangle, \tag{4}$$

which have to be solved self-consistently.

Let us first consider the case without the AB-detector. The same set-up has been studied [6] using the DMRG algorithm, which is valid even if $U$ is large (Coulomb blockade without potential barriers). There is reflection symmetry, $\langle c_1^\dagger c_1\rangle = \langle c_0^\dagger c_0\rangle$, Eqs. (3) and (4) are identical, and $V_0 = V_1 = V$. Once the self-consistent values of $v$ and $V$ are obtained, the effective transmission coefficient $t_s$ reads:

$$t_s = \frac{v\,(1 - \exp(-2ik_F))}{v^2 - \exp(-2ik_F) - 2V\exp(-ik_F) - V^2}. \tag{5}$$

For this toy model, the analytical form of $\langle c_p^\dagger c_{p'}\rangle$ of Eqs. (2,3,4) can be given as a function of $v$, $V$ and $k_F$, as in Ref. [4]. The self-consistent values of $v$ and $V$ can be obtained analytically if $U$ is small or numerically otherwise, solving the coupled Eqs. (2,3). Alternatively, one can diagonalize the HF Hamiltonian numerically for leads of finite size $N_L$, make the extrapolation to the limit $N_L \to \infty$, and numerically determine the self consistent solution of Eqs. (2,3).

Moreover, the HF-equations have a simple solution, if one makes an approximation which becomes valid when $t_d \gg 1$. We only explain the idea in this letter, the detailed calculations will be given in a forthcoming paper. The nano-system without leads and interaction has only two states of energy $V_G \pm t_d$, separated by an energy gap $2t_d$. Let us define the operators $d_s = (c_0 + c_1)/\sqrt{2}$ and $d_a = (c_0 - c_1)/\sqrt{2}$, $n_s = d_s^\dagger d_s$ and $n_a = d_a^\dagger d_a$. When $t_d$ is large and for the values of $V_G$ where $|t_s|^2 \neq 0$, the symmetric state of energy $V_G - t_d$ is below $E_F$, while the anti-symmetric state of energy $V_G + t_d$ is above $E_F$. In that case, the symmetric state is occupied ($\langle n_s\rangle \approx 1$), the anti-symmetric one is empty ($\langle n_a\rangle \approx 0$), and the solution of the HF-equations becomes straightforward. One finds $v \approx t_d + U/2$, $V \approx V_G + U/2$, and

$$|t_s|^2 \approx \Delta\left(\frac{\Gamma^2}{(V_G - V_A)^2 - \Gamma^2} - \frac{\Gamma^2}{(V_G - V_B)^2 - \Gamma^2}\right), \tag{6}$$

where $\Delta = (2t_d + U)/(2V_G + U + 2\cos k_F)$, $\Gamma = \sin k_F$, $V_A = t_d - \cos k_F$ and $V_B = -t_d - \cos k_F - U$. In FIG. 2 (B), the nano-system transmission $|t_s|^2$ without the AB-detector ($t_s$ obtained from Eq. (5)), is shown as a function of $V_G$, for 4 values of $U$, $t_d = 1$, and a Fermi momentum $k_F = \pi/8$ (filling 1/8). The corresponding number of electrons inside the nano-system $N_s = \langle n_s + n_a\rangle$ is shown above (FIG. 2 (A)). One can see that $|t_s|^2$ exhibits two peaks when $V_G$ decreases, separated by an interval $\approx 2t_d + U$, as predicted by Eq. (6). When $t_d = 1$, Eq. (6) does not give an accurate description of the effect of $V_G$, this description becoming accurate when $t_d$ is larger (see FIG. 2 (C)). $|t_s|^2 \approx 0$ when the nano-system is either empty (large positive $V_G$) or full (large negative $V_G$). Decreasing $V_G$, one has a first transmission peak when the symmetric state becomes occupied ($V_G \approx V_A$), followed by a second peak when the anti-symmetric state is filled ($V_G \approx V_B$). When $t_d < 1$, the two states become almost degenerate, they are occupied at almost the same gate voltage and the two peaks merge to form a single peak structure which is not described by Eq. (6), as shown in FIG. 2 (C).

The effect of the nano-system parameters $U$ and $V_G$ upon the leads decays as $\langle c_p^\dagger c_{p'}\rangle$ ($p' = p$ or $p+1$) towards their asymptotic values when $p \to \infty$. One finds the usual decay

$$F_{a,b,c}(p) = a + \frac{b(U, V_G)\cos(2k_F p + c(U, V_G))}{p} \tag{7}$$

of Friedel oscillations inside a 1d non interacting electron gas. This is shown in FIG. 2 (D) for $p' = p + 1$. As for $p' = p$, these decays are characterized by an asymptotic value $a$, an amplitude $b(U, V_G)$ and a phase shift $c(U, V_G)$. If one puts a one body scatterer in series with the nano-system, one can induce Friedel oscillations inside the nano-system. This will give values for the HF parameters $v$, $V_0$, $V_1 \neq V_0$ different from their values

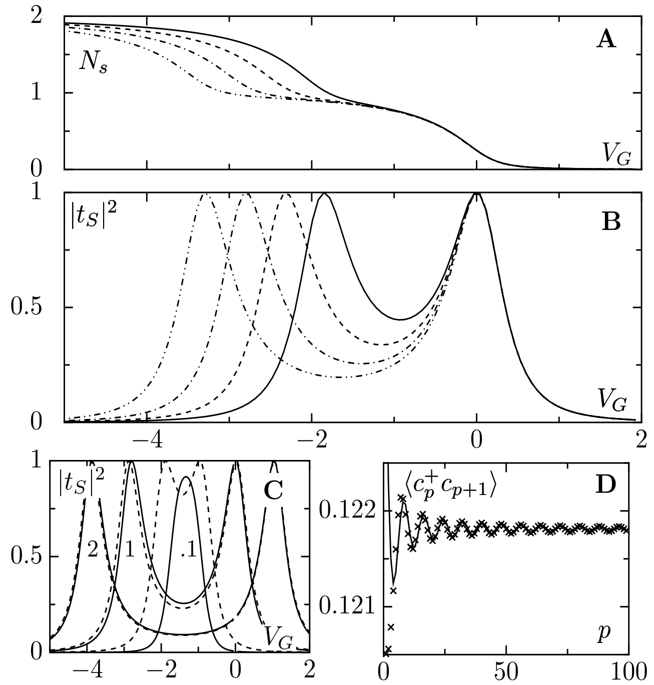


FIG. 2: Nano-system without AB-detector for $k_F = \pi/8$ (filling 1/8). A: Number $N_s$ of electrons inside the nano-system for $t_d = 1$ as a function of $V_G$ for $U = 0$ (solid), 0.5 (dashed), 1 (dot-dashed) and 1.5 (dot-dot-dashed). B: Corresponding transmission $|t_s|^2$. C: Transmission $|t_s|^2$ as a function of $V_G$ for $U = 1$ and values (2, 1 and 0.1) of $t_d$ given in the figure: exact HF behaviors (solid lines) compared to the behaviors given by Eq. (6) (dashed lines). D: $\langle c_p^\dagger c_{p+1}\rangle$ as a function of $p$ for $U = 1$ and $V_G = 0$. The solid line is an asymptotic fit $F_{a,b,c}(p)$ (Eq. (7)) of the HF values (×), with $a = 0.1218$, $b = 0.00245$ and $c = -0.38$. $\langle c_p^\dagger c_p\rangle$ (not shown) can be fitted by $F_{a,b,c}(p)$ with $a = 1/8$, $b = 0.0025$ and $c = -0.45$.

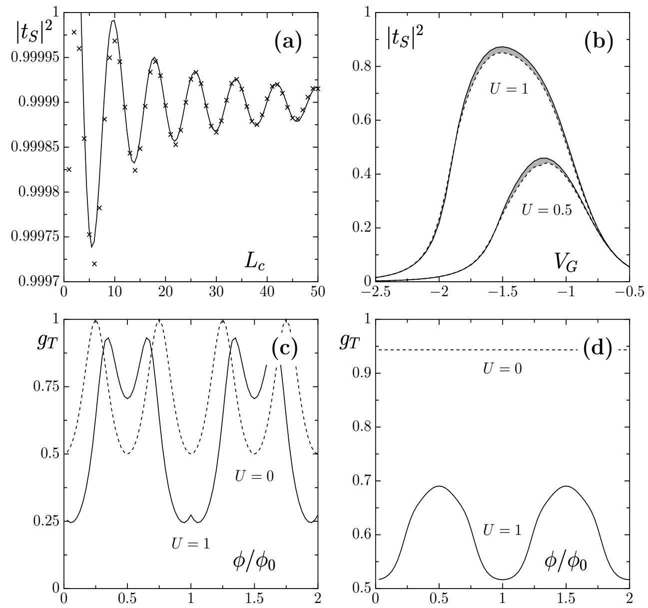


FIG. 3: Nano-system with AB-detector for $L'_c = 4$. A: Transmission $|t_s|^2$ as a function of $L_c$ for $t_d = 1$, $U = 1$, $k_F = \pi/8$, $L_R = 7$, $V_G = -2.8$ and $\Phi = 0$. HF values (×) and fit $F_{a,b,c}(p)$ (Eq. (7) - solid line) with $a = 0.9999$, $b = 0.00092$, $c = 1.678$. B: $|t_s|^2$ as a function of $V_G$ for $t_d = 0.1$, $k_F = \pi/8$, $L_R = 7$ and $L_c = 2$. The dashed (solid) curves correspond to $\Phi = 0$ ($\Phi_0/2$). The grey areas underline the effect of $\Phi$. C: Conductance $g_T$ of the nano-system and the AB-detector in series, as a function of $\Phi/\Phi_0$ for $t_d = 0.1$ and $k_F = \pi/2$. $L_c = 2$, $L_R = 7$ $V_G = -0.8$. $U = 1$ (solid line) and $U = 0$ (dashed). D: $g_T$ as a function of $\Phi/\Phi_0$ for $L_c = 2$ and $L_R = 4$ ($\sin k_F L_R = 0$). $t_d = 0.1$, $k_F = \pi/2$ and $V_g = -0.7$. $U = 1$ (solid) and $U = 0$ (dashed).

$v$, $V_0 = V_1 = V$ without the second scatterer. Using as second scatterer an AB-detector with a ring, periodic AB-oscillations of $v$, $V_0$ and $V_1$ will be induced when a flux is varied through the ring.

The AB-detector sketched in FIG. 1 includes two 3-lead contacts (3LC), the first for attaching the vertical lead to the horizontal lead, the second for attaching the ring to the vertical lead. A 3LC is made of 4 sites indicated by black circles. Its Hamiltonian is given by $H_P = -\sum_{p=1}^{3} t_{P,p}(c_P^\dagger c_p + h.c.)$, where $t_{P,p} = 1$, $P$ denoting the central site and $p$ its 3 neighbors. $L_c$ ($L'_c$) is the number of sites between the upper 3LC and the nano-system (the lower 3LC). $L_R$ is the number of sites of the ring, without those of the lower 3LC. A $3 \times 3$ matrix $S_P(k)$ describes the scattering by a 3LC at $E = -2\cos k$. $S_P(k)$ has identical diagonal elements $s_{pp} = -e^{ik}/d(k)$ and identical off-diagonal elements $s_{pp'} = (2i \sin k)/d(k) = s_{p'p}$ where $d(k) = 3e^{ik} - 2\cos k$.

The reflection amplitude of the ring (vertical lead) threaded by a flux $\Phi$ ($\varphi = 2\pi\Phi/\Phi_0$, $\Phi_0$ being the flux quantum) reads

$$r_R(\varphi) = \frac{h_k(\varphi) - \sin(kL_R)}{-h_k(\varphi) + e^{2ik}\sin(kL_R)}, \tag{8}$$

where $h_k(\varphi) = 2e^{ik}(\cos(kL_R) - \cos\varphi)\sin k$. The reflection and transmission amplitudes of the AB-detector (in the horizontal lead) read

$$r_{AB}(k) = \frac{-e^{2ik} - e^{2ikL'_c} r_R(\varphi)}{2e^{2ik} - 1 + r_R(\varphi)e^{2ik(L'_c+1)}} \tag{9}$$

$$t_{AB}(k) = \frac{2i\sin k e^{ik}(1 + e^{2ikL'_c} r_R(\varphi))}{2e^{2ik} - 1 + r_R(\varphi)e^{2ik(L'_c+1)}}. \tag{10}$$

We now study the nano-system in series with the AB-detector, solving numerically the Eqs. (2-4) for having the values $v(\varphi, L_c), V_0(\varphi, L_c)$ and $V_1(\varphi, L_c)$ characterizing the nano-system. FIG. 3 (A) shows the effect of the AB-detector upon the nano-system transmission $|t_s(L_c)|^2$, as a function of $L_c$. $t_s(L_c)$ is given by extending formula (5) to the case where $V_0 \neq V_1$. The transmission $|t_s(L_c)|^2$ exhibits decaying oscillations towards the asymptotic value characterizing the nano-system without AB-detector. The decay is given by a function $F_{a,b,c}(L_c)$.

For $t_d = 1$, the effect of the AB-detector upon $|t_s|^2$ remains negligible ($\approx 10^{-4}$), even for small values of $L_c$. This effect can be made $10^3$ times larger if $t_d$ is reduced by a factor 10. We have shown that $|t_s|^2$ is given by Eq. (6) when $t_d > 1$, in the limit where $\langle n_s \rangle \approx 1$ and $\langle n_a \rangle \approx 0$. In this limit, one cannot strongly vary $\langle n_s \rangle$ and $\langle n_a \rangle$ by the Friedel oscillations of the AB-detector, and the HF parameters are almost independent of $\varphi$. But much larger AB-oscillations of the HF parameters become possible if $t_d < 1$, when two almost degenerate levels are near $E_F$ for the same value of $V_G$. This is shown in FIG. 3 (B) for $t_d = 0.1$. The two transmission peaks shrink to form a single peak structure which depends on the flux $\varphi$ threading the ring. In FIG. 3 (B), putting $\Phi_0/2$ through the ring increases $|t_s|^2$ by a visible amount (grey areas), an effect 100 times larger than when $t_d = 1$. To make the effect even larger, one can adjust the wave-length of the Friedel oscillations to the size of the nano-system. Increasing $k_F$ from $\pi/8$ to $\pi/2$ (half-filling), the size of the AB-oscillations of $|t_s|^2$ can be increased by another factor $\approx 10$.

Having reduced the many-body scatterer to an effective one body scatterer, the conductance is given by the Landauer formula valid for a bare one body scatterer. Let us consider the two probe geometry of FIG. 1, and study the conductance $g_T$ of the nano-system and the AB-detector in series. $g_T = |t_T|^2$ (in units of $e^2/h$), where $t_T$ is given by the combination law:

$$t_T = t_s \frac{e^{ik_F L_c}}{1 - r'_s r_{AB} e^{2ik_F L_c}} t_{AB}. \tag{11}$$

$r'_s$ ($r_{AB}$) is the reflection amplitude of the nano-system (of the AB-detector). Because $r_{AB}$ and $t_{AB}$ depend on $\varphi$, $g_T$ exhibits AB-oscillations even without interaction, when $t_s$ and $r'_s$ are independent of $\varphi$ ($U = 0$ or $L_c$ too large). However, when the electrons interact inside the nano-system and $L_c$ is not too large, $t_s$ and $r'_s$ exhibit also AB-oscillations around certain values of $V_G$, which can strongly modify the AB-oscillations of $g_T$. In FIG. 3 (C), one can see how the shapes of the AB-oscillations are modified by the interaction, while their amplitudes are increased. FIG. 3 (D) corresponds to a case where the ring is perfectly reflecting at $E_F$ (Eq. (8), $r_R = -1$ when $\sin(k_F L_R) = 0$). In that special case, $t_{AB}$ and $r_{AB}$ are independent of $\varphi$ at $E_F$. But $g_T$ does have AB-oscillations when the electrons interact inside the nano-system, the HF corrections depending on HF states below $E_F$ for which $\sin(k_\alpha L_R) \neq 0$. In this special case, the very large AB-oscillations of $g_T$ are a pure many body effect.

The effect of the flux upon the HF parameters can be also detected if one uses 4 probes instead of 2. The idea [7] is to weakly contact 2 additional probes near the nano-system, for measuring directly the voltage drop at its extremities, and not on a larger scale including the AB-detector. However, since our effect requires to have the nano-system and the AB-detector inside the same quantum coherent region, the obtained conductance is no longer given by the 2 probe formula $g_s = |t_s|^2$, but by the multi-terminal formula [8] derived by Büttiker. In a 4 probe set-up, this formula yields also non local effects without interaction, which have been observed in mesoscopic conductors, using metallic wires [9] or semiconductor nanostructures [10], where the interaction is too weak for making our many body effect important. But the non local effect seen in Refs. [9, 10] should be strongly enhanced, if a region where the electrons interact is included between the 2 voltage probes.

We have studied spinless fermions (polarized electrons) and 1d leads, and shown that an attached ring can considerably modify the nano-system transmission for well chosen values of $U$, $V_G$, $t_d$ when $L_c$ is not too large. The HF approximation could be easily extended to higher dimensions. To include the spins could be more difficult. The double occupancy of each site becoming possible, a Hubbard repulsion must be added, making our double site model slightly more complicated than the Anderson model used for the Kondo problem [11]. The study of the effect of flux dependent Friedel oscillations upon the Kondo problem is left for future investigations.

We thank G. Faini, M. Sanquer and specially D. Weinmann for useful comments. The support of the network "Fundamentals of nanoelectronics" of the EU (contract MCRTN-CT-2003-504574) is gratefully acknowledged.

---

[1] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle systems* (McGraw Hill, 1971).
[2] Y. Imry, *Introduction to Mesoscopics Physics* (Oxford University Press, 2002).
[3] R. A. Molina, D. Weinmann, and J.-L. Pichard, Eur. Phys. J. B **48**, 243 (2005).
[4] Y. Asada, A. Freyn, and J.-L. Pichard, Eur. Phys. J. B **53**, 109 (2006).
[5] C. Kittel, *Quantum Theory of Solids* (John Wiley and Sons, 1963).
[6] G. Vasseur, D. Weinmann, and R. A. Jalabert, Eur. Phys. J. B **51**, 267 (2006).
[7] H.-L. Engquist and P. W. Anderson, Phys. Rev. B **24**, 1151 (1981).
[8] M. Büttiker, Phys. Rev. Lett. **57**, 1761 (1986).
[9] S. Washburn, in *Mesoscopic Phenomena in Solids*, edited by B. L. Alsthuler, P. A. Lee, and R. A. Webb (North Holland, 1991).
[10] W. J. Skocpol, P. M. Mankiewich, R. E. Howard, L. D. Jackel, D. M. Tennant, and A. D. Stone, Phys. Rev. Lett. **58**, 2347 (1987).
[11] A. C. Hewson, *The Kondo Problem To Heavy Fermions* (Cambridge University Press, 1993).